Local Density of States in the Antiferromagnetic and Ferromagnetic Kondo Models

P. Sinjukow,[1,*] D. Meyer,[1,2] and W. Nolting[1]

[1] *Lehrstuhl Festkörpertheorie, Institut für Physik, Humboldt-Universität zu Berlin, Invalidenstr. 110, 10115 Berlin, Germany*
[2] *Department of Mathematics, Imperial College, 180 Queen's Gate, London SW7 2BZ, UK*

(Dated: February 1, 2008)

Based on a simple approximation scheme we have computed the local density of states (LDOS) of the antiferromagnetic and ferromagnetic Kondo models for the full range of band occupations and coupling strengths. For both models the LDOS with its full energy dependence has not been calculated before. Arguments are given for the results to be qualitatively trustworthy despite the simplicity of the approximation scheme.

I. INTRODUCTION

The term *antiferromagnetic Kondo model* stands for the well-known single-impurity *Kondo model*, whose origin is ascribed to Zener[1]. The attribute *antiferromagnetic* is used to stress the difference to the *ferromagnetic Kondo model*. In both models the spin of a magnetic impurity is coupled to the spins of the conduction electrons of a non-magnetic host lattice. In the (antiferromagnetic) Kondo model the sign of the coupling constant is such that antiparallel coupling between the impurity and the conduction-electron spins is favoured (antiferromagnetic intraatomic exchange). In the ferromagnetic Kondo model, with the opposite sign of the coupling constant, parallel coupling is favoured (ferromagnetic intraatomic exchange).

The (antiferromagnetic) Kondo model has been one of the most intensively discussed many-body models in solid state physics since Kondo in 1964 succeeded in explaining the resistance minimum of metals with small amounts of transition element impurities[2]. Thorough theoretical investigations later on led to the discovery of the cause of the minimum, the Kondo effect, which is the collective (many-body) screening of the impurity spin by the spins of the conduction electrons below the Kondo temperature T_K[3,4]. By means of Wilson's numerical renormalization group theory (NRG)[5] and Bethe-ansatz methods[6,7] exact solutions for thermodynamic properties such as the magnetic susceptibility and the heat capacity were obtained. Later the NRG was successfully extended to the computation of dynamic (energy-dependent) quantities[8,9,10].

Although the antiferromagnetic Kondo model can thus be regarded as in principle solved, its local density of states (LDOS) with the full energy dependence has not been calculated so far[11]. Nevertheless the LDOS is an interesting quantity, particularly since scanning tunneling spectroscopy (STS) has made it experimentally accessible[12,13,14,15].

The LDOS of the ferromagnetic Kondo model, too, has not been calculated yet. The ferromagnetic Kondo model has generally received less attention than its antiferromagnetic counterpart. This is probably due to the fact that a spectacular "ferromagnetic Kondo effect" does not exist because the effective coupling does not scale to infinity as in the antiferromagnetic Kondo model[3,4]. A second reason might be that there are fewer experimental realizations than in the antiferromagnetic case.

In this paper we present results for the $T = 0$-LDOS of both the antiferromagnetic and the ferromagnetic Kondo models for the full range of band occupations and coupling strengths, gained by means of a simple Green's function approximation scheme based on Nagaoka's decoupling procedure[16]. The equations of Nagaoka's decoupling scheme were solved analytically by Zittartz and Müller-Hartmann[17]. However, their equations still depend self-consistently on the scattering matrix. Therefore, in order to find self-consistent numerical solutions, it is equally well justified to use Nagaoka's original equations.

Qualitatively results prove trustworthy despite the crudness of the approximations. For weak couplings the main correlation feature in the impurity-site LDOS of the antiferromagnetic Kondo model is an antiresonance, which is slightly shifted with respect to the Fermi level. There is an analogous antiresonance in the LDOS of the single-impurity Anderson model. A related antiresonance structure was observed in recent STS measurements on magnetic impurity adatoms[13,14,15]. For strong couplings the dominant characteristic are quasiparticle δ-peaks. These can be traced back to the limiting case of an empty conduction band, for which exact results and rigorous interpretation are given, and the atomic limit[18].

In the ferromagnetic Kondo model the LDOS at the Fermi level is practically independent on the coupling strength, which is consistent with the fact of a vanishing phase shift. However, the LDOS is diminished in the vicinity, giving rise to a peak-like structure. If representing a true feature, this peak structure should be measurable in STS experiments on magnetic adatoms with *ferromagnetic* intraatomic exchange.

It is clear that the approximation scheme is too simple to yield quantitatively reliable results. Subtle features like the exponential Kondo scale in the antiferromagnetic Kondo model cannot be reproduced. Much better methods like numerical renormalization group theory (NRG) or Quantum Monte Carlo (QMC)[19] would be required

*Electronic address: peter.sinjukow@physik.hu-berlin.de

for that.

This paper is structured as follows: First the exact solution for the limiting case of an empty conduction band (Sec. II A) and the approximation scheme for finite band occupation (II B) are explained. Then the results for the LDOS are discussed in detail: first, for the case of an empty conduction band (III A), which is similar in both models, second, for the case of finite band occupation in the antiferromagnetic Kondo model (III B), and third, for finite band occupations in the ferromagnetic Kondo model (III C). After that the influence of the magnetic impurity on occupation numbers is discussed with emphasis on a seemingly contradictory result by other authors (III D). Finally we draw some conclusions (IV).

II. THEORY

The Hamiltonian of the antiferromagnetic and ferromagnetic Kondo models is given by

$$\mathcal{H} = \sum_{ij\sigma} T_{ij} c^\dagger_{i\sigma} c_{j\sigma} - J\,\mathbf{S}_0 \cdot \boldsymbol{\sigma}_0 \quad . \tag{1}$$

Replacing $\boldsymbol{\sigma}_0$ by Fermi operators yields

$$\mathcal{H} = \sum_{ij\sigma} T_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \frac{J}{2} \sum_{\sigma} (z_\sigma S^z_0 n_{0\sigma} + S^\sigma_0 c^\dagger_{0-\sigma} c_{0\sigma}) \tag{2}$$

with $z_\sigma = \delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}$ and $S^\sigma_0 = \delta_{\sigma\uparrow} S^+_0 + \delta_{\sigma\downarrow} S^-_0$. The first part of $\mathcal{H}$ with the hopping integrals T_{ij} describes the free movement of conduction electrons in a nondegenerate band. $c^{(\dagger)}_{i\sigma}$ annihilates (creates) an electron in a spin-σ Wannier state at the lattice site $\mathbf{R}_i$. The second part stands for the interaction between the impurity spin $\mathbf{S}_0$ and the spins of the conduction electrons represented by $\boldsymbol{\sigma}_0$. Throughout this paper a spin-$\frac{1}{2}$ impurity will be considered. We assume a k-independent coupling constant J. Therefore the coupling is effectively local, involving only electrons at the impurity site $\mathbf{R}_0$. $\mathcal{H}$ represents the (antiferromagnetic) Kondo model if $J < 0$, and the ferromagnetic Kondo model for $J > 0$.

A. Exact solution for an empty conduction band

Appropriate Fourier transformations of the equations of motion for the Green's functions $G_{ij\uparrow}(E) = \langle\!\langle\, c_{i\uparrow}\,;\, c^\dagger_{j\uparrow}\,\rangle\!\rangle_E$ and $\Gamma_{0ij\uparrow}(E) = \langle\!\langle\, S^z_0 c_{i\uparrow}\,;\, c^\dagger_{j\uparrow}\,\rangle\!\rangle_E$ lead to the following closed system of equations:

$$G_{jj\uparrow} = G^{(0)}_{00} - G^{(0)}_{j0} \frac{3}{2} J\, \Gamma_{00j\uparrow} \tag{3}$$

$$G_{0j\uparrow} = G^{(0)}_{00} - G^{(0)}_{00} \frac{3}{2} J\, \Gamma_{00j\uparrow} \tag{4}$$

$$\Gamma_{00j\uparrow} = -G^{(0)}_{00} \frac{J}{8} G_{0j\uparrow} + G^{(0)}_{00} \frac{J}{2} \Gamma_{00j\uparrow} \quad . \tag{5}$$

The free Green's functions are given by $G^{(0)}_{ij}(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}}{E - \epsilon(\mathbf{k}) + i0^+}$, with N the number of lattice sites. Solving (3) – (5) yields the solution:

$$G_{jj\uparrow} = G^{(0)}_{00} - \frac{G^{(0)}_{00} \frac{3}{16} J^2 \big(G^{(0)}_{j0}\big)^2}{\big(G^{(0)}_{00}\big)^2 \frac{3}{16} J^2 + G^{(0)}_{00} \frac{1}{2} J - 1} \quad . \tag{6}$$

With (6), the LDOS $\rho_{j\uparrow}$ of any given site $\mathbf{R}_j$ can be calculated: $\rho_{j\uparrow}(E) = -\frac{1}{\pi} \mathrm{Im} G_{jj\uparrow}(E)$. The spin dependence of $\rho_{j\uparrow}$ is purely formal.

For our calculations we have chosen the tight-binding dispersion with nearest-neighbour hopping for the s.c. lattice:

$$\epsilon(\mathbf{k}) = -2t(\cos k_x a + \cos k_y a + \cos k_z a) \tag{7}$$

where t is the hopping integral and a the lattice constant. (7) implies a symmetric Bloch density of states (BDOS) and $\mathrm{Im} G^{(0)}_{i0}(E) = \pm \mathrm{Im} G^{(0)}_{i0}(-E)$, which result in a mirror symmetry of the LDOS when changing from the antiferromagnetic to the ferromagnetic Kondo model: $\rho^{(J)}_{i\uparrow}(E) = \rho^{(-J)}_{i\uparrow}(-E)$ at any site $\mathbf{R}_i$.

B. Approximation scheme for finite band occupation

For $G_{ij\uparrow}$ Eqs. (3) and (4) remain correct. For $\Gamma_{0ij\uparrow}$ two new Green's functions come into play, to which Nagaoka's decoupling scheme is applied[16]. Consequently, Eq. (5) is replaced by

$$\begin{aligned} &\Gamma_{00j\uparrow}(E) \approx \\ &\approx \Big(- G^{(0)}_{00}(E) \frac{J}{8} + J \langle\, S^z_0 c^\dagger_{0\uparrow} \tilde{c}_{0\uparrow}(E)\,\rangle \Big)\, G_{0j\uparrow}(E) \\ &+ \Big(G^{(0)}_{00}(E) \frac{J}{2} - J \langle\, c^\dagger_{0\uparrow} \tilde{c}_{0\uparrow}(E)\,\rangle \Big)\, \Gamma_{00j\uparrow}(E) \,. \end{aligned} \tag{8}$$

We have defined special energy-dependent annihilation operators

$$\tilde{c}_{0\sigma}(E) \stackrel{\text{def.}}{=} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\mathbf{R}_0}}{E - \epsilon(\mathbf{k}) + i0^+}\, c_{\mathbf{k}\sigma} \tag{9}$$

to avoid multiple k-space summations within the self-consistency cycle of this approximation scheme. The remaining problem is to determine the correlation functions of Eq. (8). They are complex quantities, whose real and imaginary parts must be determined separately via the spectral theorem with the help of appropriately defined operators and Green's functions. For example:

$$\mathrm{Re} \langle\, c^\dagger_{0\uparrow} \tilde{c}_{0\uparrow}(E)\,\rangle = \langle\, c^\dagger_{0\uparrow} \overset{R}{\tilde{c}}_{0\uparrow}(E)\,\rangle \tag{10}$$

$$\text{with} \quad \overset{R}{\tilde{c}}_{0\sigma}(E) \stackrel{\text{def.}}{=} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathcal{P} \frac{e^{i\mathbf{k}\mathbf{R}_0}}{E - \epsilon(\mathbf{k})}\, c_{\mathbf{k}\sigma} \,, \tag{11}$$

$\mathcal{P}$ meaning "principal part of". One needs

$$\overset{R}{G}_{00\uparrow}(E,E') = \langle\!\langle\ \overset{R}{c}_{0\uparrow}(E)\,;\, c_{0\uparrow}\ \rangle\!\rangle_{E'} \tag{12}$$

with E a parameter and E' the usual energy variable of the Green's function to determine $\langle\, c^\dagger_{0\uparrow}\, \overset{R}{c}_{0\uparrow}(E)\,\rangle$ via the spectral theorem

$$\langle\, c^\dagger_{0\uparrow}\, \overset{R}{c}_{0\uparrow}(E)\,\rangle = -\frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\mathrm{Im}\overset{R}{G}_{00\uparrow}(E,E')}{e^{\beta(E'-\mu)}+1}dE' \ . \tag{13}$$

Comparing the respective equations of motion for $\overset{R}{G}_{00\uparrow}(E,E')$ and $G_{00\uparrow}(E)$ one can show that $\overset{R}{G}_{00\uparrow}(E,E')$ is fully determined by the "simple" one-electron Green's function through

$$\overset{R}{G}_{00\uparrow}(E,E') = \ \frac{\overset{R}{G}^{(0)}_{00}(E,E')}{G^{(0)}_{00}(E')}\, G_{00\uparrow}(E')\ , \tag{14}$$

with

$$\overset{R}{G}^{(0)}_{00}(E,E') = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{E'-\epsilon(\mathbf{k})+i0^+}\mathcal{P}\frac{1}{E-\epsilon(\mathbf{k})}\,. \tag{15}$$

Thus $\mathrm{Re}\langle\, c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$ and, analogously, $\mathrm{Im}\langle\, c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$ are fully determined by $G_{00\uparrow}$.

To determine the real part of the other correlation function, $\mathrm{Re}\langle\, S^z_0 c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$, one needs the Green's function $\overset{R}{\Gamma}_{000\uparrow}(E,E') = \langle\!\langle\ S^z_0\, \overset{R}{\tilde{c}}_{0\uparrow}(E)\,;\, c^\dagger_{0\uparrow}\ \rangle\!\rangle_{E'}$. We assume the same proportionality (14) that holds between $\overset{R}{G}_{00\uparrow}(E,E')$ and $G_{00\uparrow}(E')$ for the Γ-Green's functions:

$$\overset{R}{\Gamma}_{000\uparrow}(E,E') \approx \ \frac{\overset{R}{G}^{(0)}_{00}(E,E')}{G^{(0)}_{00}(E')}\,\Gamma_{000\uparrow}(E')\ \ . \tag{16}$$

Note that Eq. (16) is required to work only within the spectral-theorem integration over E' to determine $\mathrm{Re}\langle\, S^z_0 c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$. Within that integration great contributions arise for $E' \approx E$, for which (16) can be shown to be reasonably justified. Analogous considerations can be made for $\mathrm{Im}\langle\, S^z_0 c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$.

Hence, one has a closed system of equations consisting of (3), (4), (8), (14), (16), the analogues to (14) and (16) for determining $\mathrm{Im}\langle\, c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$ and $\mathrm{Im}\langle\, S^z_0 c^\dagger_{0\uparrow}\tilde{c}_{0\uparrow}(E)\,\rangle$, and the spectral theorems (such as (13)) for the real and imaginary parts of the correlation functions. The LDOS $\rho_{i\uparrow}(E) = -\frac{1}{\pi}\mathrm{Im}G_{ii\uparrow}(E)$ can be self-consistently determined for any lattice site $\mathbf{R}_i$. The spin dependence of $\rho_{j\uparrow}$ is purely formal. The occupation number at $\mathbf{R}_i$ is gained by integrating over the LDOS:

$$\langle n_i\rangle = 2 * \int_{-\infty}^{+\infty} dE\ \frac{\rho_{i\uparrow}(E)}{e^{\beta(E-\mu)}+1}\ . \tag{17}$$

III. RESULTS AND DISCUSSION

A. LDOS in the limiting case of an empty conduction band

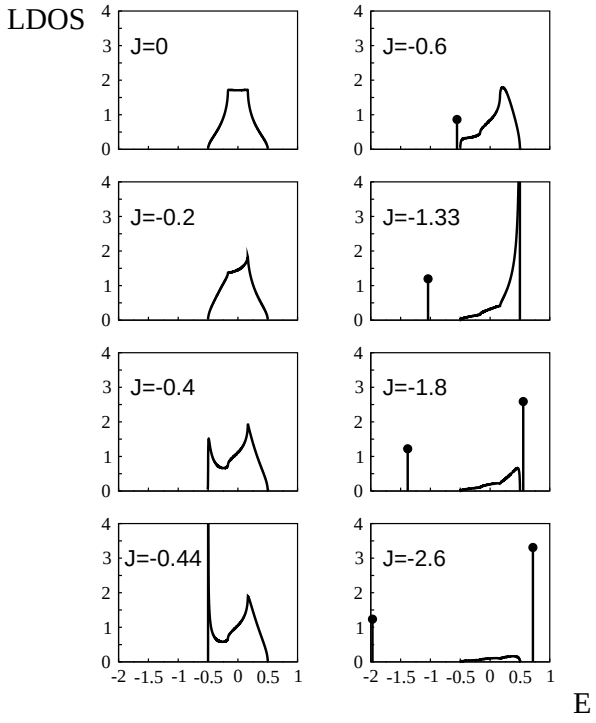

FIG. 1: LDOS of the antiferromagnetic Kondo model at the impurity site in the limiting case of an empty conduction band for various values of the coupling constant J. δ-peaks are represented by pins whose heights are proportional to the corresponding spectral weights. The free Bloch dispersion is given by Eq. (7). The energy is measured in units of the bandwidth.

We first discuss the limiting case of an empty conduction band, in which results are exact and allow rigorous interpretation, and which is similar in the antiferromagnetic and ferromagnetic Kondo models. The LDOS represents the outcome of an inverse-photoemission experiment in which one test-electron is put into the empty conduction band. It thus provides information on the impurity's effects on one-electron states. In Figs. 1 and 2 the LDOS of the antiferromagnetic Kondo model at the impurity and the nearest-neighbour sites is shown for various coupling constants $J < 0$. The LDOS of the ferromagnetic Kondo model ($J > 0$) is simply given by the mirror image of the LDOS of the antiferromagnetic Kondo model with the same $|J|$. This symmetry is a consequence of the Bloch dispersion we have chosen (Eq. (7)). A general dispersion gives similar but not exactly symmetric results for the two models.

At $J = 0$ the LDOS corresponds to the free Bloch density of states (BDOS). Small couplings cause deformations of the LDOS, most pronounced at the impurity site. For $J < -0.44$ there appears a δ-peak below,

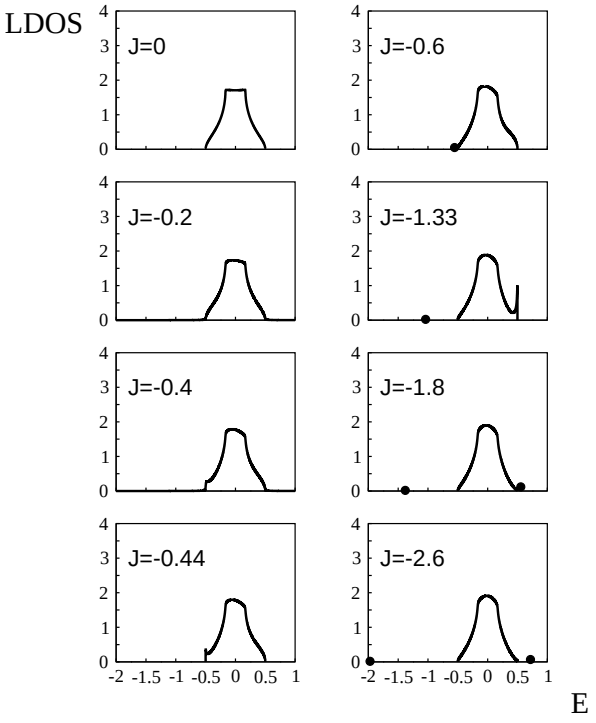

FIG. 2: LDOS of the antiferromagnetic Kondo model at a nearest-neighbour site of the impurity in the limiting case of an empty conduction band. The rest as in Fig. 1.

for $J < -1.33$ a second δ-peak above the quasiparticle band. The upper peak has greater spectral weight than the lower. At the nearest-neighbour site the weight of both peaks is considerably less than at the impurity site. With increasing $|J|$ the peaks move away from the quasiparticle band. At the impurity site their weight increases, while the weight of the quasiparticle band gradually vanishes. At the neighbouring site the δ-peaks lose weight (not recognizable in Fig. 2) and the quasiparticle band approaches a certain asymptotic form.

This can be well understood from the strong-coupling limit ($J \to -\infty$). In that limit the singlet and triplet states with the electron completely localized at the impurity site are energy eigenstates. The other one-electron states are extended band states, deformed in the vicinity of and zero at the impurity site, thereby meeting the condition of orthogonality to the fully localized states. Therefore, in the strong-coupling limit the LDOS at the impurity site consists of two δ-peaks, their positions tending towards $-\infty$ and $+\infty$, corresponding to the diverging energies of the bound singlet and triplet states. The quasiparticle band has zero weight as there is no overlap of the band states to the impurity site. At the other sites the LDOS vice versa consists of a quasiparticle band only. It is deformed because the probability of the electron to stay at the respective site is redistributed between and within the extended states.

For finite J the bound states have finite overlaps to the neighbouring sites of the impurity, which is reflected

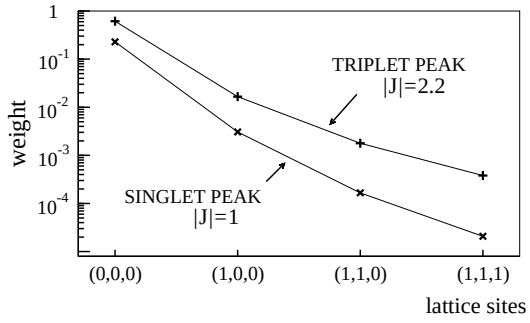

FIG. 3: Quasi-exponential decrease of the spectral weights of the singlet and triplet peaks with increasing distance from the impurity site (0,0,0). The weight of the singlet peak is shown for $|J| = 1$, the weight of the triplet peak for $|J| = 2.2$. (Calculated for same Bloch dispersion as in Fig. 1.)

by quasiparticle δ-peaks with small but finite weights. Since the eigenstates with one electron can be classified as pure singlet or triplet states for all J, the lower and upper quasiparticle δ-peaks correspond to bound singlet and triplet states, respectively. The greater weight of the upper peak ("triplet peak") results from the degeneracy of the triplet states. The degree of localization of the bound states around the impurity site is very large as can be seen when comparing the spectral weights of the singlet and triplet peaks at the impurity and neighbouring sites (Fig. 3). There is a quasi-exponential decrease of weights/overlaps with increasing distance from the impurity. The extended band states in case of finite J have a finite overlap to the impurity site, which is reflected by the finite weight of the quasiparticle band in the impurity-site LDOS.

If considering singlet and triplet states separately, the situation is similar to the quantum-mechanical problem of a particle in a potential landscape with a well or barrier. For instance, the bound singlet state corresponds to a bound state in a potential well, which has an exponentially decreasing overlap into the adjacent region if the depth of the well is finite. In case of an infinitely deep well, corresponding to the strong-coupling limit, each bound state is restricted to the well while the extended states have no overlap into the well region.

For large values of J the effect of the hopping from and to the impurity site becomes negligible compared to the spin-spin coupling. Therefore, as far as the impurity site is concerned, a comparison with the atomic limit[18] is sensible. In case of zero band occupation the LDOS in the atomic limit consists of two quasiparticle δ-peaks whose positions are at $+\frac{3}{4}J$ (singlet) and $-\frac{1}{4}J$ (triplet), having spectral weights of $\frac{1}{4}$ and $\frac{3}{4}$, respectively. In Fig. 4 it is shown how the weights and positions of the singlet and triplet peaks in the impurity-site LDOS converge for large J towards the corresponding atomic-limit values, which confirms the emergence of fully localized (atomic) states in the strong-coupling limit.

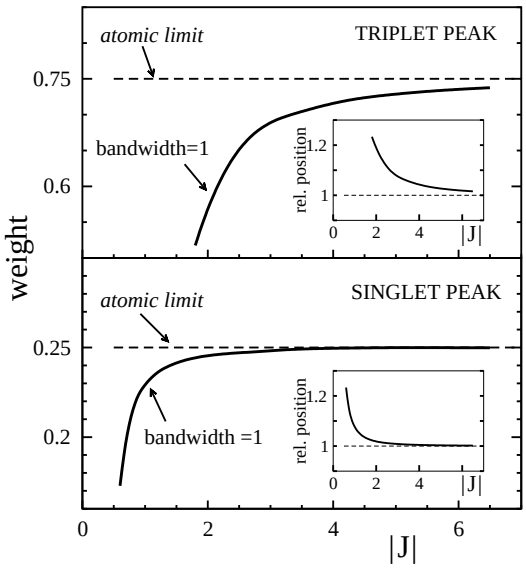

FIG. 4: Convergence of the weights and positions of the impurity-site singlet and triplet peaks toward the respective atomic-limit values. The solid lines in the insets show the *relative positions* of the peaks (ratio of position in bandwidth=1-case and atomic limit). (Calculated for same Bloch dispersion as in Fig. 1.)

B. LDOS in the antiferromagnetic Kondo model

In Fig. 5 our results for the Kondo-model LDOS at the impurity site for different band occupations n and the full range of weak to strong couplings J are presented. At more than half filling ($n > 1$) the LDOS is simply given by the mirror image of the corresponding LDOS at a band occupation of $2 - n$ (due to particle-hole symmetry of the Kondo Hamiltonian (1) and the selection of a symmetric free BDOS). For weak to intermediate couplings ($|J| \leq 0.4$) and not too small band occupations ($n \geq 0.2$) the most prominent feature in the LDOS is an antiresonance at the Fermi level, which will be discussed in subsection 1. In the strong-coupling regime ($|J| \geq 0.6$) quasiparticle δ-peaks are the dominant characteristic, which are discussed in subsection 2.

1. *Kondo antiresonance*

For small couplings ($J = -0.1$) the LDOS exhibits a narrow, dip-like structure at the Fermi level. When increasing the coupling strength ($J = -0.2, -0.4$) it deepens and broadens, developing into a marked antiresonance. As shown in Fig. 6, the antiresonance appears not exactly at the Fermi energy but is slightly shifted (upward shift for $n < 1$). For strong couplings ($|J| \geq 0.6$) the LDOS at the Fermi level is practically zero. However, no antiresonance in the narrower sense is left, instead the LDOS is dominated by quasiparticle peaks. In the following paragraphs we will discuss independent evidence for an antiresonance in the (antiferromagnetic) Kondo model. After that, the antiresonance will be related to a structure recently observed in STS experiments.

In Ref. 20 Mezei and Zawadowski considered the Kondo model for different types of scattering. They made explicit statements on the LDOS for the resonance energy, for which they could refer to a definite value of the phase shift. For s-type scattering they found complete suppression of the LDOS, while non-s-type scattering was shown to involve no changes at the resonance energy. As each of the scattering types (s, p, etc.) is connected with a special wave-vector dependence in the coupling constant, it seems a priori unclear how to apply those results to the Kondo model with a wave-vector independent coupling-constant J discussed in this paper.

Evidence for an antiresonance in the LDOS of the Kondo model is provided by a comparison with results for the (single-impurity) Anderson model[21]. As is well-known, the Anderson model in the so-called Kondo limit can be mapped on the Kondo model by the unitary Schrieffer-Wolff transformation[22]. A correspondence must be expected between results in the Kondo limit of the Anderson model and the weak-coupling limit of the Kondo model. In the Anderson model one does observe an antiresonance in the conduction-electron LDOS. It is closely related to the appearance of the well-known Kondo resonance (peak) in the impurity quasiparticle density of states (impurity QDOS). Sollie and Schlottmann calculated the conduction-electron LDOS and the impurity QDOS of the single-impurity Anderson model within the slave-boson approach[23]. The conduction-electron LDOS shows the antiresonance appearing at the same energy and with the same width as the Kondo resonance in the impurity QDOS, which reveals the intimate relation between both structures. Both appear not exactly at the Fermi energy but slightly above, similar to what we observe for the antiresonance in the Kondo model. More recently Schiller and Hershfield emphasized the direct correspondence between antiresonance and Kondo resonance ("Abrikosov-Suhl resonance") in the Anderson model[24].

We have performed a calculation for the Anderson model within the modified perturbation theory (MPT). The MPT is an extension of the conventional second-order perturbational scheme[4,26] to improve the strong-coupling behaviour away from the symmetric point, which is the only point at which the conventional perturbation theory also converges for large Hubbard interaction U.[27] For details we refer to Ref. 28, where the MPT was successfully applied to the single-impurity Anderson model. It has also been used in the context of the dynamical mean-field theory (DMFT) to examine the Hubbard model[29] and the periodic Anderson model[30,31]. Our results for the single-impurity Anderson model for three different band occupations n are shown in Fig. 7. The Kondo resonance in the impurity QDOS and the antiresonance in the conduction-electron LDOS are clearly to be seen at the Fermi level (for $n = 0.2$, 0.6 slightly above).

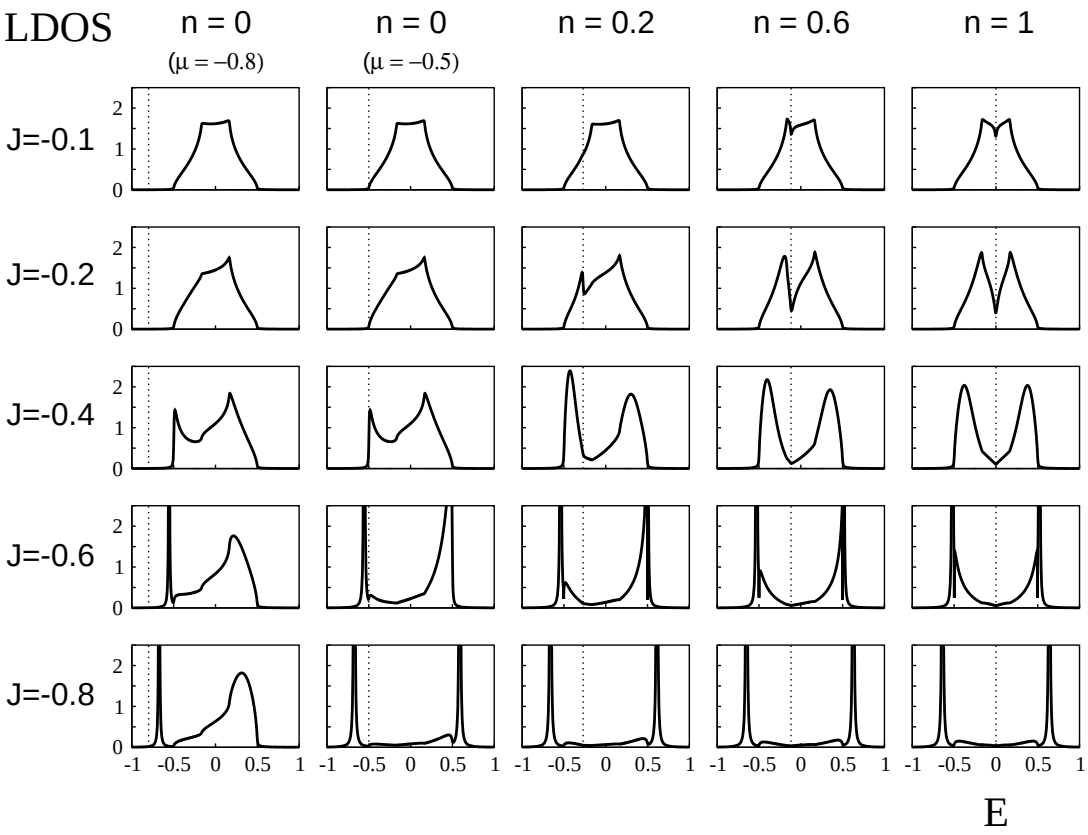

FIG. 5: LDOS of the antiferromagnetic Kondo model at the impurity site for various coupling constants J and band occupations n. The position of the chemical potential μ is indicated by the thin dotted line. The narrow resonances outside the quasiparticle band are quasiparticle δ-peaks. (Calculation for the same Bloch dispersion as in Fig. 1.)

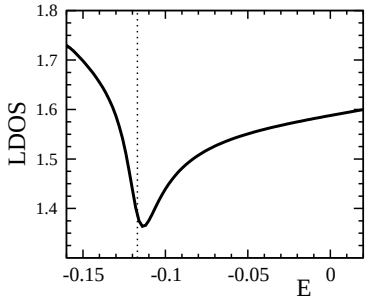

FIG. 6: Antiresonance in the impurity-site LDOS of the antiferromagnetic Kondo model ($n = 0.6$, $J = -0.1$). The Fermi level is indicated by the thin dotted line. The shift of the antiresonance relative to the Fermi level is of the order of 10^{-3} in units of the bandwidth. (Same calculation as in Fig. 5.)

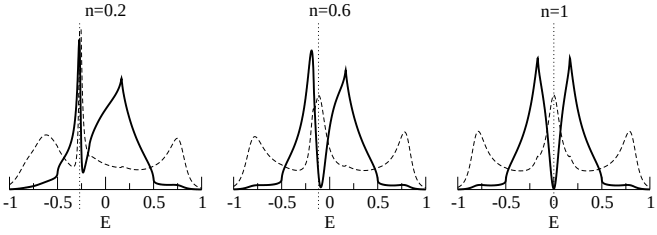

FIG. 7: Conduction-electron LDOS at impurity site (solid line) and impurity QDOS (broken line) in the Anderson model for different band occupations n calculated with the modified perturbation theory (MPT). The position of the Fermi level is indicated by the thin dotted line. Parameters: $U = 1$, $V = 0.2$ (Bloch dispersion as in Fig. 5).

With the parameters chosen, an approximate correspondence to the Kondo model with $J = -0.16$ is to be expected according to the Schrieffer-Wolff transformation. For each of the three band occupations the Anderson-model LDOS is indeed quite similar to the Kondo-model LDOS for $J = -0.2$ in Fig. 5. The only basic difference is for the symmetric Anderson-model LDOS, where the antiresonance goes right down to zero, whereas in the $n = 1$ Kondo-model LDOS it does not. For the symmetric Anderson model one can show, using the fact that the electrons form a Fermi liquid, that the conduction-electron LDOS of the impurity site must be zero at the Fermi energy. Assuming this is conserved in the Schrieffer-Wolff transformation, it is apparently a shortcoming of our approximation scheme that for small to intermediate couplings the symmetric Kondo-model LDOS is not fully suppressed at the Fermi energy. Furthermore, one cannot expect our approximation scheme to satisfy the

subtle exponential dependence of the width of the antiresonance on the coupling constant J via the Kondo temperature T_K[4], which should occur in analogy to the Anderson model. Nevertheless, the antiresonances coming out from the calculations clearly indicate the correct antiresonance of the Kondo model. Since the antiresonance of the Kondo model is closely connected with the one in the Anderson model and because of the intimate relation of the latter to the well-known Kondo resonance, we use for both antiresonance structures the term "Kondo antiresonance".

Recently experimental evidence was found for the Kondo antiresonance in the conduction-electron LDOS of magnetic impurity adatoms on metal surfaces. In scanning tunneling spectroscopy (STS) experiments the differential conductance dI/dV was measured for the cases of Ce adatoms on a Ag(111) surface[13], for Co on Au(111)[14] and for Co on Cu(111)[15]. In each experiment a narrow antiresonance structure with a slight upward shift relative to the Fermi level was observed in the dI/dV spectrum. Following Ref. 24, in case of weak tunneling, low enough temperatures ($T \to 0$) and in an energy range in which the LDOS of the STM tip is nearly constant, the differential conductance dI/dV is in general proportional to what we shall call a "mixed LDOS". Contributions to this "mixed LDOS" come from all electronic states ("tunneling channels") of the substrate that are involved in the tunneling process. The "mixed LDOS" is not just the sum over partial densities of states but also contains quantum-interference effects between the different tunneling channels.

As for their measurements on Ce/Ag(111), Li et al. assumed that they were "locally sensitive to the hybridized *sp* conduction band"[13]. This is supported by Schiller and Hershfield[24], who achieved optimal theoretical agreement with the measured antiresonance curve on the assumption that alternative tunneling into the impurity (Ce) f-orbital was zero. Accordingly, the pure conduction-electron LDOS was probed, which allows to directly identify the antiresonance in the dI/dV spectrum with the Kondo antiresonance in the conduction-electron LDOS.

By contrast, in the case of Co/Au(111) the involvement of the tunneling channels and the interpretation of the dI/dV spectrum are a matter of controversy. Madhavan et al. assumed significant contributions from tunneling both into the conduction band and the impurity d-orbital of the Co adatom, attributing an asymmetry of the antiresonance to quantum-interference effects between the d-orbital and the conduction electron channels[14]. This was confirmed by an excellent theoretical fit of the antiresonance. However, Újsághy et al. assumed tunneling into the conduction band only and achieved an equally good theoretical fit[25]. The ambiguity is already inherent in Fano's theory[32], which in Refs. 14 and 25 was generalized to the interacting case. For non-interacting electrons one can show that the asymmetric shape of a "Fano resonance" depends, first, on the ratio of tunneling into the impurity orbital and tunneling into the conduction band, and secondly, on the symmetry/asymmetry of the free conduction-electron BDOS and the Fermi-level position. Each of these factors and combinations of the two can lead to the same line shape. This seems to hold in the present (interacting) case, too. We conclude that in the case of Co/Au(111) the dI/dV spectrum possibly represents a direct measure of the conduction-electron LDOS. If so, the asymmetric antiresonance (Fano resonance) directly represents a Kondo antiresonance. If not, a Kondo antiresonance may still be considered as the main underlying structure apart from impurity-orbital contributions and quantum-interference effects.

2. Quasiparticle δ-peaks

In the strong-coupling regime ($|J| \geq 0.6$) the LDOS of the Kondo model is dominated by quasiparticle δ-peaks. In Fig. 5 they appear as narrow resonances. For the limiting case of an empty conduction band (Sec. III A) we have discussed the emergence of a singlet and a triplet peak, corresponding to the excitation of bound one-electron singlet and triplet eigenstates through inverse photoemission. With increasing J first the singlet peak emerges from the quasiparticle band. In Fig. 5 this can be seen again in the first column on the left, which represents the limiting case of an empty conduction band. If the singlet peak is present, one has to distinguish another case of zero band occupation $n = 0$ (second column in Fig. 5), characterized by the chemical potential μ lying between the singlet peak and the quasiparticle band. In this case there is exactly one electron in the system, occupying the bound singlet state, *before* the excitation in inverse or direct photoemission. With this electron the band occupation n (i.e. the average number of electrons per lattice site) is still zero, but the physical situation differs from "the limiting case of an empty conduction band". This is reflected by the drastic differences between the corresponding LDOS's in Fig. 5.

For certain values of the coupling constant (cf. $J = -0.6$) the emergence of a second quasiparticle peak can be triggered by increasing the band occupation. The generic situation of the strong-coupling regime is the presence of two quasiparticle peaks. In the case of half filling they are positioned symmetrically above and below the quasiparticle band, whose weight gradually vanishes with increasing coupling strength (cf. $J = -0.6, -0.8$). The LDOS for large J approaches the LDOS of the atomic limit, which for $n = 1$ consists of two symmetric singlet peaks[18], the lower one observable in direct, the upper in inverse photoemission. The quasiparticle peaks of the strong-coupling regime clearly correspond to the singlet peaks of the atomic limit. Nevertheless, in the present case of finite hopping, admixtures of triplet coupling at the impurity site are to be expected, which only disappear in the limit $J \to \infty$. Note that these would not contradict the overall singlet nature of the Kondo-model ground state. In Ref. 23 similar quasipar-

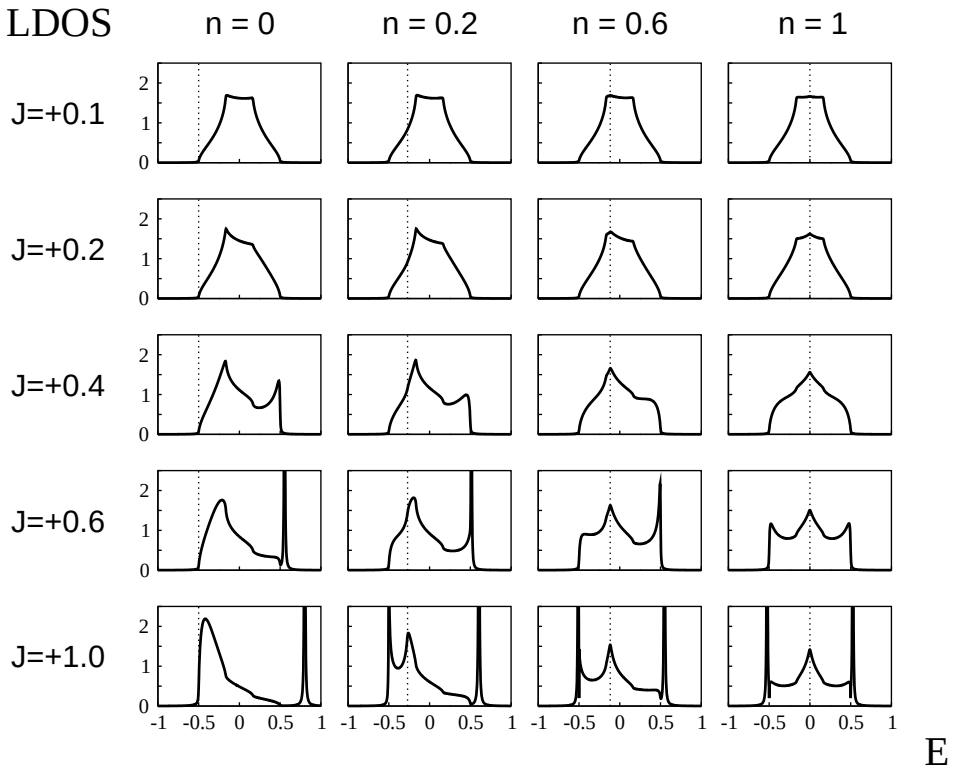

FIG. 8: LDOS of the ferromagnetic Kondo model at the impurity site for various coupling constants J and band occupations n. The position of the chemical potential is indicated by the thin dotted line. The narrow resonances outside the quasiparticle band are quasiparticle δ-peaks. (Calculation for the same Bloch dispersion as in Fig. 1.)

ticle peaks close to the band edges were observed in the conduction-electron LDOS of the single-impurity Anderson model.

C. LDOS in the ferromagnetic Kondo model

Figure 8 shows our results for the impurity-site LDOS in the ferromagnetic Kondo model for low to strong couplings J and different band occupations n. Due to particle-hole symmetry, it is sufficient to consider band occupations up to half filling. The most remarkable feature is a peak structure at the position of the Fermi level. Note that the peak structure is not a true resonance — in the sense that the LDOS is not really enhanced at the maximum in comparison to the free BDOS. This agrees with what one should expect because of the vanishing phase shift at the Fermi level in the ferromagnetic Kondo model. Instead, compared to the BDOS the LDOS is diminished in the vicinity of the maximum position. The peak structure is slightly shifted relative to the Fermi level (Fig. 9) similar to the Kondo antiresonance of the antiferromagnetic Kondo model.

If the peak structure at the Fermi level is a true feature of the ferromagnetic Kondo model, it should in principle be detectable in an STS experiment similar to the Kondo antiresonance (cf. Sec. III B 1). In an STS measurement the differential conductance dI/dV represents a direct measure of the conduction-electron LDOS on condition that tunneling occurs only into the conduction band. The peak structure in the LDOS of the ferromagnetic Kondo model should thus be observable as a seeming enhancement in the differential conductance near the Fermi level. However, the preparation of adatoms with *ferromagnetic* exchange ($J > 0$) is required. Gd adatoms might be suitable candidates since in bulk Gd the intraatomic exchange is ferromagnetic, which can be inferred from an excess $T = 0$ magnetic moment due to induced "ferromagnetic" spin-polarisation of $5d-6s$ conduction electrons[33].

As in the antiferromagnetic Kondo model, for sufficiently large couplings J quasiparticle δ-peaks appear, whose emergence can partly be triggered by increasing the band occupation (cf. $J = 0.1$). Again, the generic situation in the strong-coupling regime is the presence of two quasiparticle δ-peaks. In case of half filling they are located symmetrically below and above the quasiparticle band, whose weight gradually vanishes when increasing the coupling strength. Similar to the antiferromagnetic Kondo model and the limiting case of an empty conduction band, the LDOS in the strong-coupling regime should approach the LDOS of the atomic limit. The two symmetric quasiparticle δ-peaks therefore correspond to the two triplet peaks in the atomic limit[18] of the ferro-

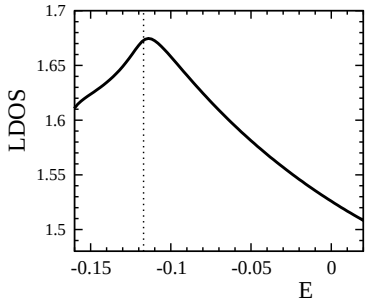

FIG. 9: Peak structure in the impurity-site LDOS of the ferromagnetic Kondo model ($n = 0.6$, $J = +0.2$). The Fermi level is indicated by the thin dotted line. The shift of the peak structure relative to the Fermi level is of the order of 10^{-3} in units of the bandwidth. (Same calculation as in Fig. 8.)

magnetic Kondo model for $n = 1$. Nevertheless, in the case of finite hopping, admixtures of singlet character are to be expected, which only disappear in the limit $J \to \infty$. The assumption of singlet admixtures is supported by the observation that for $J = 1.0$ the upper peak in the $n = 1$-LDOS continuously evolves from the pure singlet peak of the $n = 0$-LDOS (limiting case of an empty conduction band) when changing the band occupation from 0 to 1.

D. Occupation numbers

In Fig. 10 the effect of the magnetic impurity on the occupation number $\langle n_0 \rangle$ at the impurity site is demonstrated. Depending on the band occupation n, the impurity can effectively attract or repel the conduction electrons both in the antiferromagnetic and ferromagnetic Kondo models. For a symmetric BDOS the dependence on the band occupation is exactly symmetric: below half filling the impurity effectively attracts the conduction electrons, $\langle n_0 \rangle - n > 0$ for $-0.5 < \mu < 0$, above half filling it repels them, $\langle n_0 \rangle - n < 0$ for $0 < \mu < 0.5$.

The physical reason for this behaviour is clear and should analogously hold for a non-symmetric BDOS. One of the possible couplings of an electron to the impurity spin (in the antiferromagnetic Kondo model the singlet, in the ferromagnetic Kondo model the triplet) decreases the energy of the system, making it favourable for the electron to stay at the impurity site. Thus, $\langle n_0 \rangle$ is increased compared to the band occupation n in the case of less than half filling. However, it is unfavourable for a second electron to be at the impurity site (since it would break the favourable coupling of the other electron), which leads to an occupation number less than the band occupation in the case of more than half filling. In a generalized form this argument implies a critical band occupation above which the occupation number at the impurity site is less than in the rest of the lattice, corresponding to a repulsive effect of the impurity on the conduction electrons. Below we discuss results of Refs. 34 and 35 which are seemingly contradictory to this.

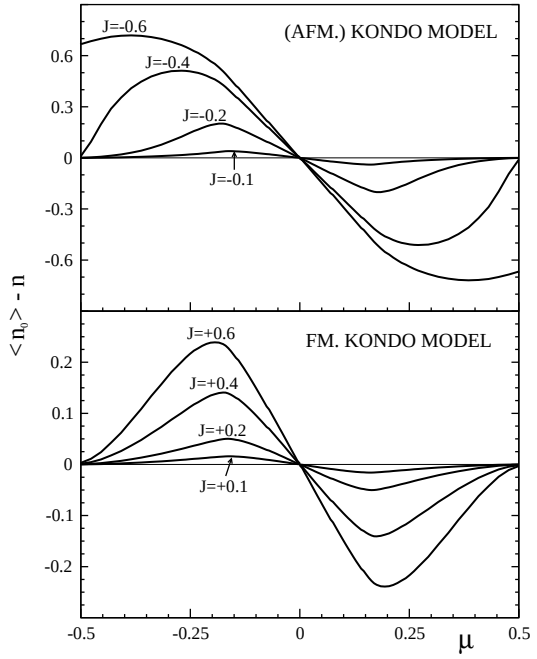

FIG. 10: Difference between the occupation number at the impurity site and the band occupation, $\langle n_0 \rangle - n$, in dependence on the Fermi level μ for different values of the coupling constant J. $\mu = -0.5$ corresponds to zero band-occupation, $\mu = 0$ to half filling and $\mu = +0.5$ to a completely filled band. (Calculated for same Bloch dispersion as in Fig. 1.)

The effect of the magnetic impurity on the occupation numbers $\langle n_i \rangle$ at the surrounding lattice sites is demonstrated in Fig. 11. Oscillations around the value of the band occupation which decrease in amplitude with growing distance from the impurity are to be seen. The oscillations in the occupation number reflect the Friedel oscillations in the charge density, which are the typical reaction of an electron system to an impurity potential. Everts and Ganguly derived an expression for the charge density in the Kondo model (Ref. 34). Šokčević, Zlatić and Horvatić calculated charge-density oscillations in the Anderson model (Ref. 35). A quantitative comparison between charge-density and occupation-number results is only partly possible. The occupation number is the number of electrons in the Wannier states at a given lattice site, whereas the charge density corresponds to the number of electrons per unit volume for a given point of space. In contrast to the occupation number, the charge density at and near a site depends also on electrons in Wannier states of other sites because in real space Wannier wave-functions are not confined to "their" sites. Although there is no rigorous proportionality between occupation number and charge density, one should, nevertheless, expect correlations between the two as far as general features such as oscillations or pronounced enhancements/reductions are concerned.

In view of such general correlations it may seem unclear why in in the cited references the charge density at the

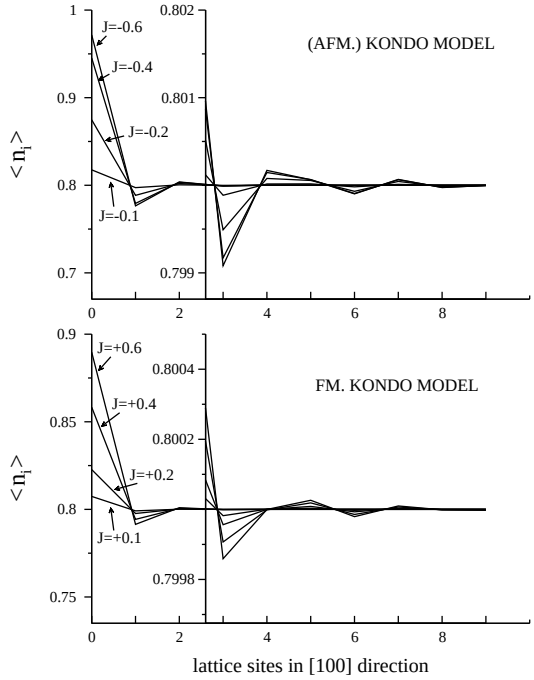

FIG. 11: Oscillations in the occupation number $\langle n_i \rangle$ for successive lattice sites in the [100] direction at a band occupation of $n = 0.8$ for different coupling constants J. (Calculation for s.c. lattice with same Bloch dispersion as in Fig. 1.)

impurity is *always enhanced* (even divergent) independent of the band occupation or k_F, ϵ_F etc. It seemingly contradicts our above argument. However, the result of permanent enhancement of the charge density at the impurity site is non-generic and a consequence of integrations without cut-off. Integrations were performed over plane waves up to arbitrarily large wave vectors. Thus an infinite number of bands is implied with each one-electron state coupled to the impurity spin with practically the same coupling strength. There is no critical band occupation in this effective infinite-band model because an arbitrarily large number of electrons can stay at the impurity being coupled to its spin in a favourable way.

IV. CONCLUSIONS

We have provided results for the local density of states (LDOS) in the antiferromagnetic and ferromagnetic Kondo models, which has not been calculated before with its full energy dependence. Although calculations were performed within a simple approximation scheme, results prove at least in qualitative terms trustworthy, allowing consistent interpretation and qualitative comparison with the experiment. There are clear quantitative limitations as indicated for example by the insufficient depth of the Kondo antiresonance. Nevertheless, we would expect confirmation of the general features by quantitatively reliable methods like NRG or QMC.

In summary, for small to intermediate couplings there is an antiresonance in the LDOS of the antiferromagnetic Kondo model (Kondo antiresonance), which has an analogue in the conduction-electron LDOS of the Anderson model. The Kondo antiresonance can be identified with antiresonance structures observed in STS spectra of single magnetic adatoms on the assumption that tunneling occured mainly into the conduction band. In the ferromagnetic Kondo model a peak structure appears close to the Fermi level. It should be observable in appropriate STS experiments on adatoms with ferromagnetic intraatomic exchange (possibly Gd adatoms). For strong couplings the LDOS in both models is dominated by quasiparticle δ-peaks, which can be clearly related to the quasiparticle peaks of the exactly solvable case of an empty conduction band and the atomic limit. Finally, we have given arguments for the impurity's attractive or repulsive effect on conduction electrons at the impurity site dependent on the band occupation and for seemingly contradictory results gained by integrating without band cut-off.

Acknowledgments

We would like to thank W. Hofstetter for drawing our attention to Refs. 13,14,15. We acknowledge the support of the DFG (Sonderforschungsbereich 290) and the Volkswagen Foundation. One of us (D. M.) gratefully acknowledges the support of the Friedrich-Naumann Foundation.

[1] C. Zener, Phys. Rev. **81**, 440 (1951).
[2] J. Kondo, Prog. Theor. Phys **32**, 37 (1964).
[3] A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. **32**, 453 (1983).
[4] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1997).
[5] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[6] N. Andrei, Phys. Rev. Lett. **45**, 379 (1980).
[7] P. B. Wiegmann, Sov. Phys. JETP Lett. **392**, 1980 (1980).
[8] H. O. Frota and L. N. Oliviera, Phys. Rev. B **33**, 7871 (1986).
[9] O. Sakai, Y. Shimizu, and T. Kasuya, J. Phys. Soc. Japan

58, 3666 (1989).
[10] T. A. Costi, A. Hewson, and V. Zlatić, J. Phys.: Condens. Matter **6**, 2519 (1994).
[11] In Ref. 20 Mezei and Zawadowski derived analytical expressions for the Kondo-model LDOS for different types of scattering in terms of an energy-dependent phase shift. However, they made explicit statements on only one energy point, for which they could refer to a definite value of the phase shift.
[12] M. F. Crommie, C. P. Lutz, and D. M. Eigler, Phys. Rev. B **48**, 2851 (1993).
[13] J. Li, W.-D. Schneider, R. Berndt, and B. Delley, Phys. Rev. Lett. **80**, 2893 (1998).
[14] V. Madhavan, W. Chen, T. Jamneala, M. F. Crommie, and N. S. Wingreen, Science **280**, 567 (1998).
[15] H. C. Manoharan, C. P. Lutz, and D. M. Eigler, Nature **403**, 512 (2000).
[16] Y. Nagaoka, Phys. Rev. **138**, A 1112 (1965).
[17] J. Zittartz, and E. Müller-Hartmann Z. Phys. **212**, 380 (1968).
[18] W. Nolting and M. Matlak, phys. stat. sol. (b) **123**, 155 (1984).
[19] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[20] F. Mezei and A. Zawadowski, Phys. Rev. B **3**, 167 (1971).
[21] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[22] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).
[23] R. Sollie and P. Schlottmann, Phys. Rev. B **42**, 6099 (1990).
[24] A. Schiller and S. Hershfield, Phys. Rev. B **61**, 9036 (2000).
[25] O. Újsághy, J. Kroha, L. Szunyogh, and A. Zawadowski, Phys. Rev. Lett. **85**, 2557 (2000).
[26] K. Yosida and K. Yamada, Suppl. Prog. Theor. Phys. **46**, 244 (1970).
[27] V. Zlatić and B. Horvatić, Phys. Rev. B **28**, 6904 (1983).
[28] D. Meyer, T. Wegner, M. Potthoff, and W. Nolting, Physica B **270**, 225 (1999).
[29] M. Potthoff, T. Wegner, and W. Nolting, Phys. Rev. B **55**(24), 16132 (1997).
[30] D. Meyer and W. Nolting, Phys. Rev. B **61**, 13465 (2000).
[31] D. Meyer and W. Nolting, Phys. Rev. B **62**, 5657 (2000).
[32] U. Fano, Phys. Rev. **124**, 1866 (1961).
[33] L. W. Roeland, G. J. Cock, F. A. Muller, C. A. Moleman, K. A. M. Mc Ewen, R. C. Jordan, and D. W. Jones, J. Phys. F **5**, L233 (1975).
[34] H. U. Everts and B. N. Ganguly, Phys. Rev. **174**, 594 (1968).
[35] D. Šokčević, V. Zlatić, and B. Horvatić, Phys. Rev. B **39**, 603 (1989).